# Advancing Materials Modeling to Accelerate Net Shape Fabrication

## Current Status and Future Vision

Kris Wise
NASA LaRC

# Incubator Capability Target

A tool for on-demand fabrication of net shape, multifunctional components for aerospace structural applications.

Meeting this target will require significant advances in:

- Printer technology
- CNT fiber reinforced feedstock
- *<u>Methods for optimally designing the components to leverage advances in printer and feedstock</u>*

# Why a New Design Method?

Current design methods were created for:

- Metals – subtractive manufacturing
- Composites – sheet/tape prepreg layup manufacturing
- Plastics – molding and extrusion processes

New materials and fabrication process permit:

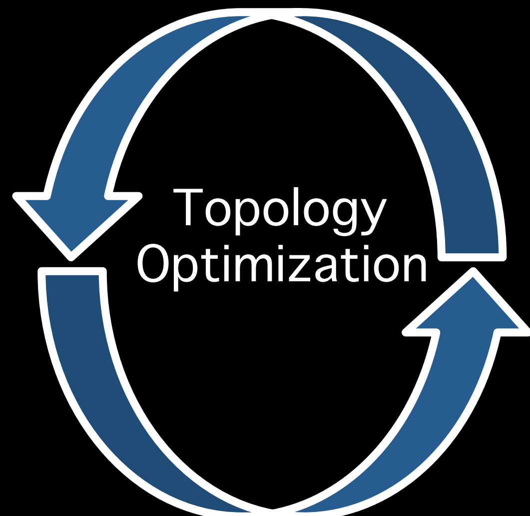
- Optimizing placement/orientation of CNT reinforcement
- Balancing stiffness/strength with mass reduction
- Incorporating electrical and thermal conductivity paths
- Optimizing tool paths for fabrication

*Existing design tools cannot do what is required*

# Topology Optimization

Topology Optimization is an automated technique for optimally designing structures subject to prescribed performance targets and boundary conditions

Structural Design




Material Selection
And Placement

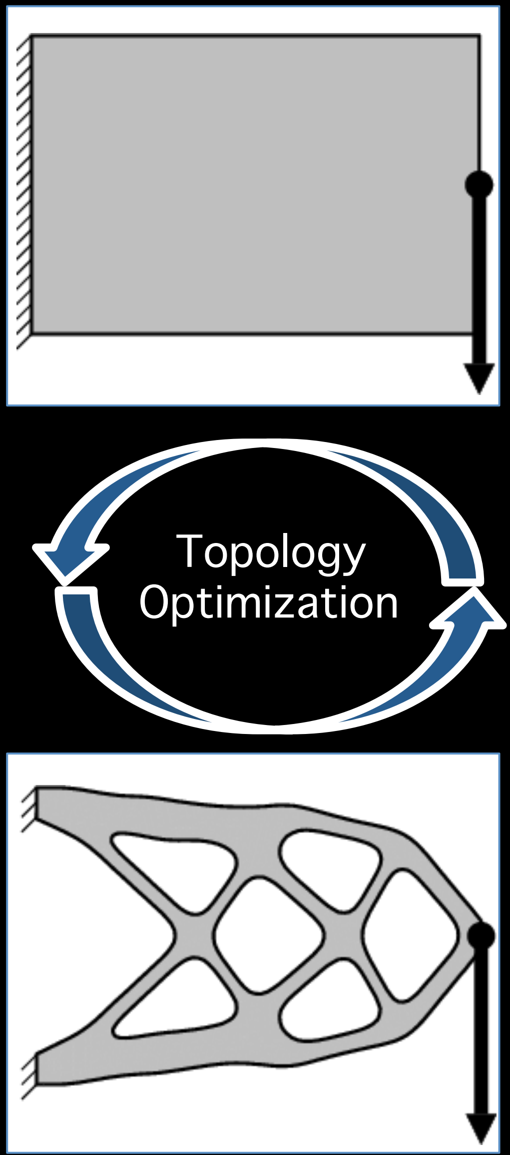
## Input

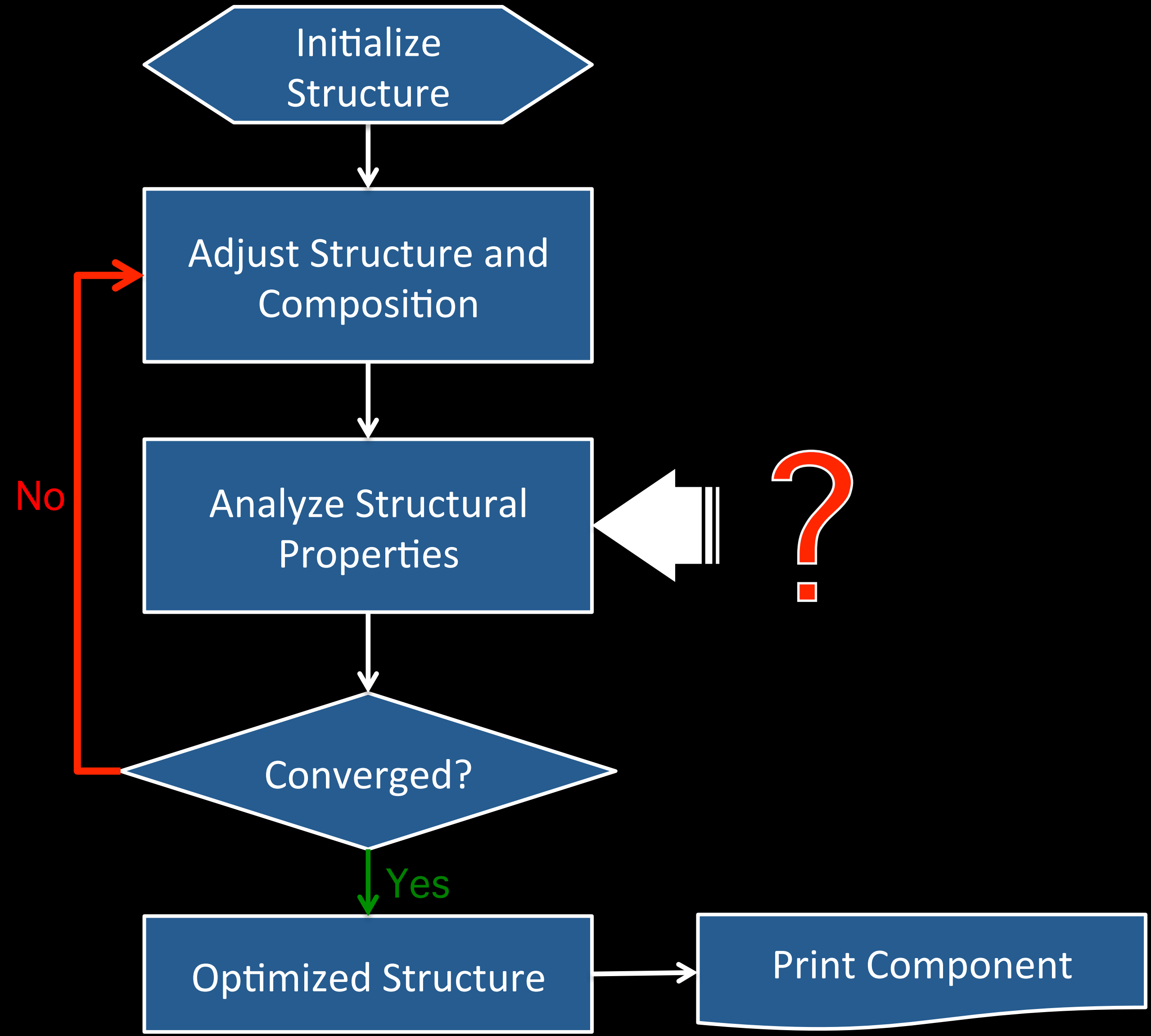
- Loading Requirements
- Mass Constraints
- Dimensional Boundaries
- Material(s) Properties

## Output

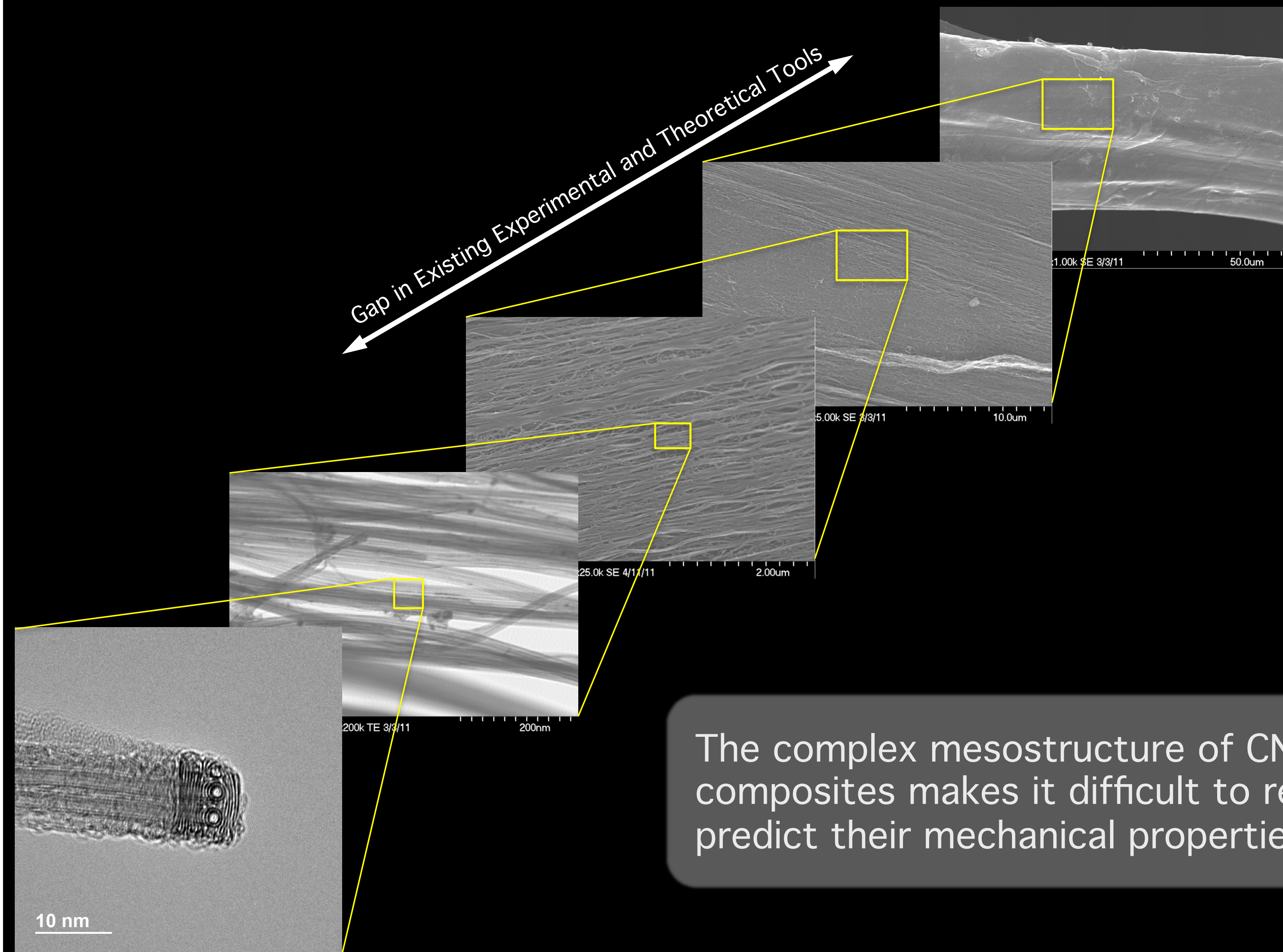
- Component Shape
- Material Distribution
- Loading Capacity
- Response Properties

# Topology Optimization Flow Chart

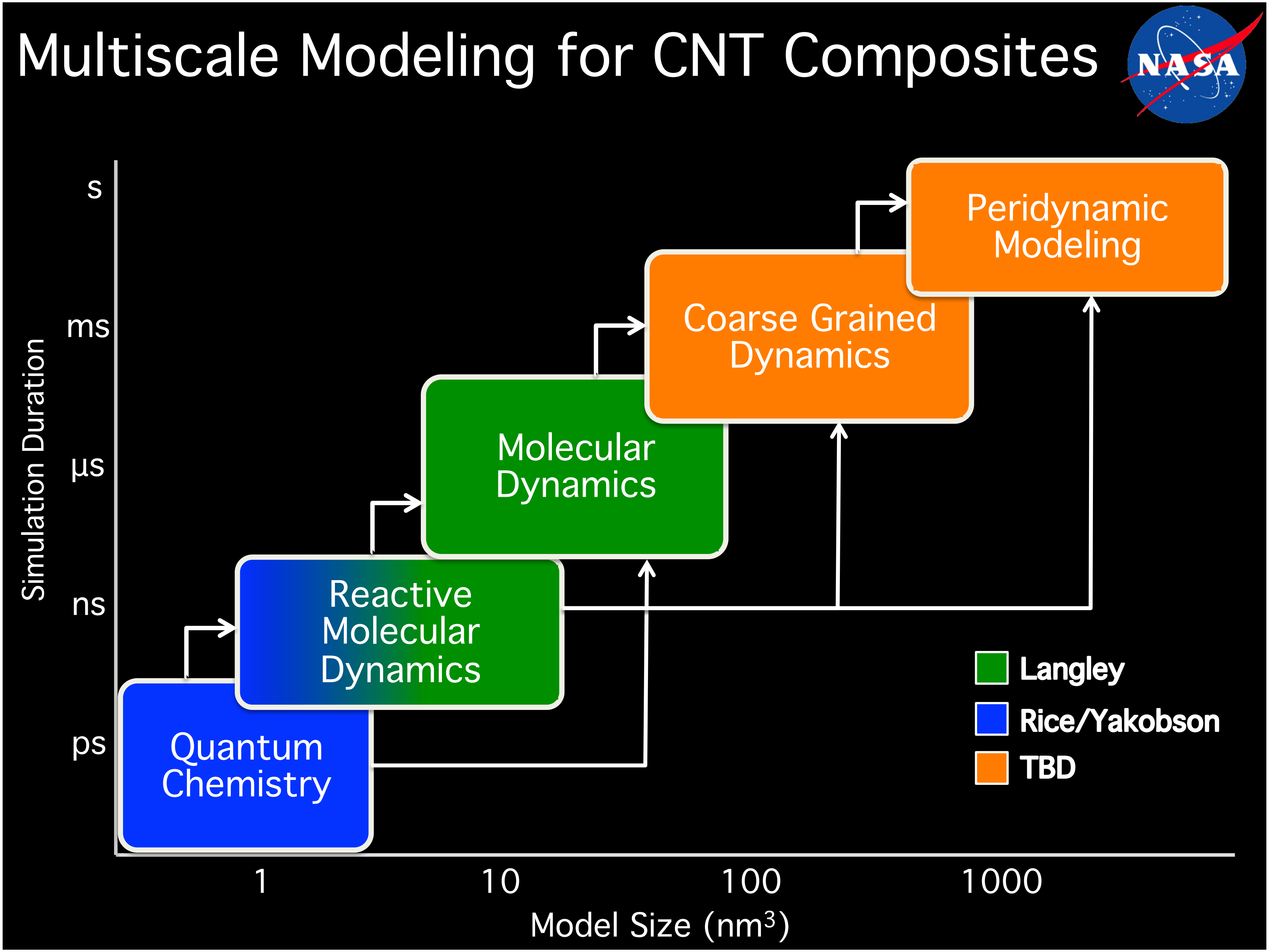


# Multiscale Structure of CNT Fibers




The complex mesostructure of CNT composites makes it difficult to reliably predict their mechanical properties


Multiscale Modeling for CNT Composites
NASA
Simulation Duration
s
ms
µs
ns
ps
Peridynamic Modeling
Coarse Grained Dynamics
Molecular Dynamics
Reactive Molecular Dynamics
Quantum Chemistry
Langley
Rice/Yakobson
TBD
1
10
100
1000
Model Size (nm³)

# What is Peridynamic Modeling?

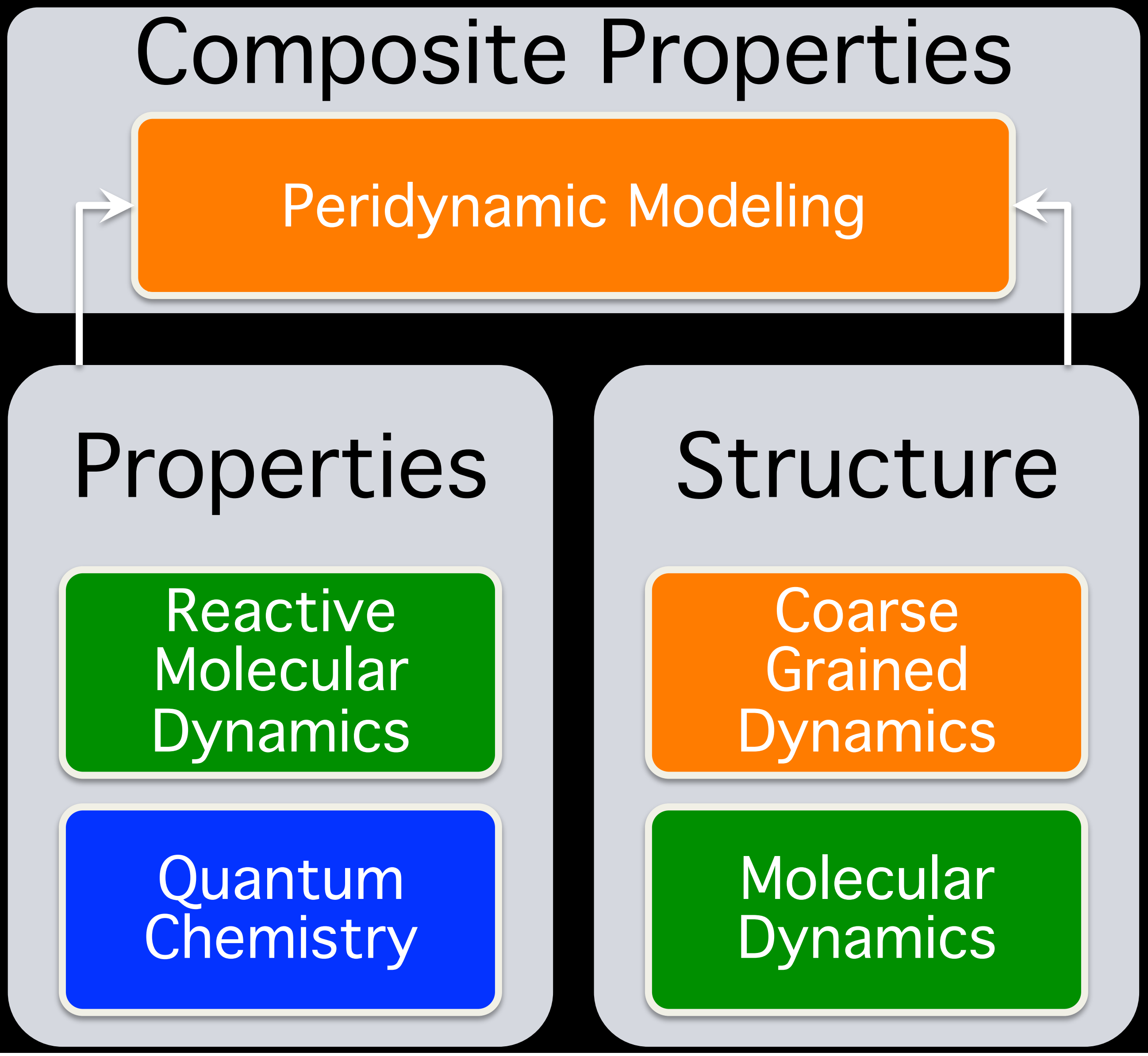
## A recent method with exciting capabilities:

- Introduced in 2000, still in active development
- Represents continuum materials with material points
- Nonlocal theory that bridges from finite element to molecular dynamics via an adjustable internal length parameter

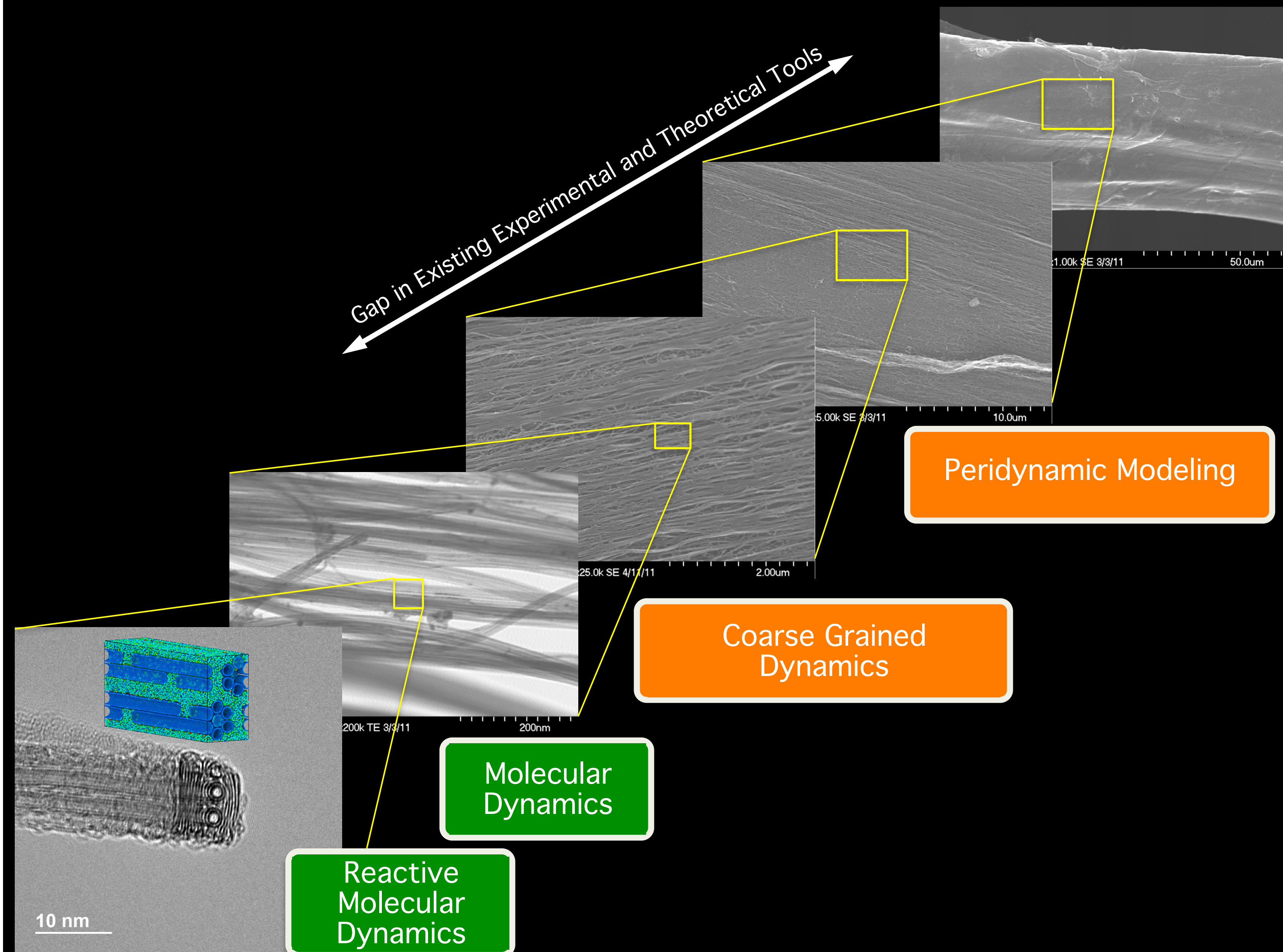
## Particularly for CNT fiber composite materials:

- Damage initiation and propagation at multiple sites
- Arbitrary fracture paths without special crack growth criteria
- Permits arbitrary numbers and shapes of inclusions and voids
- Material properties depend on detailed micro/mesostructure

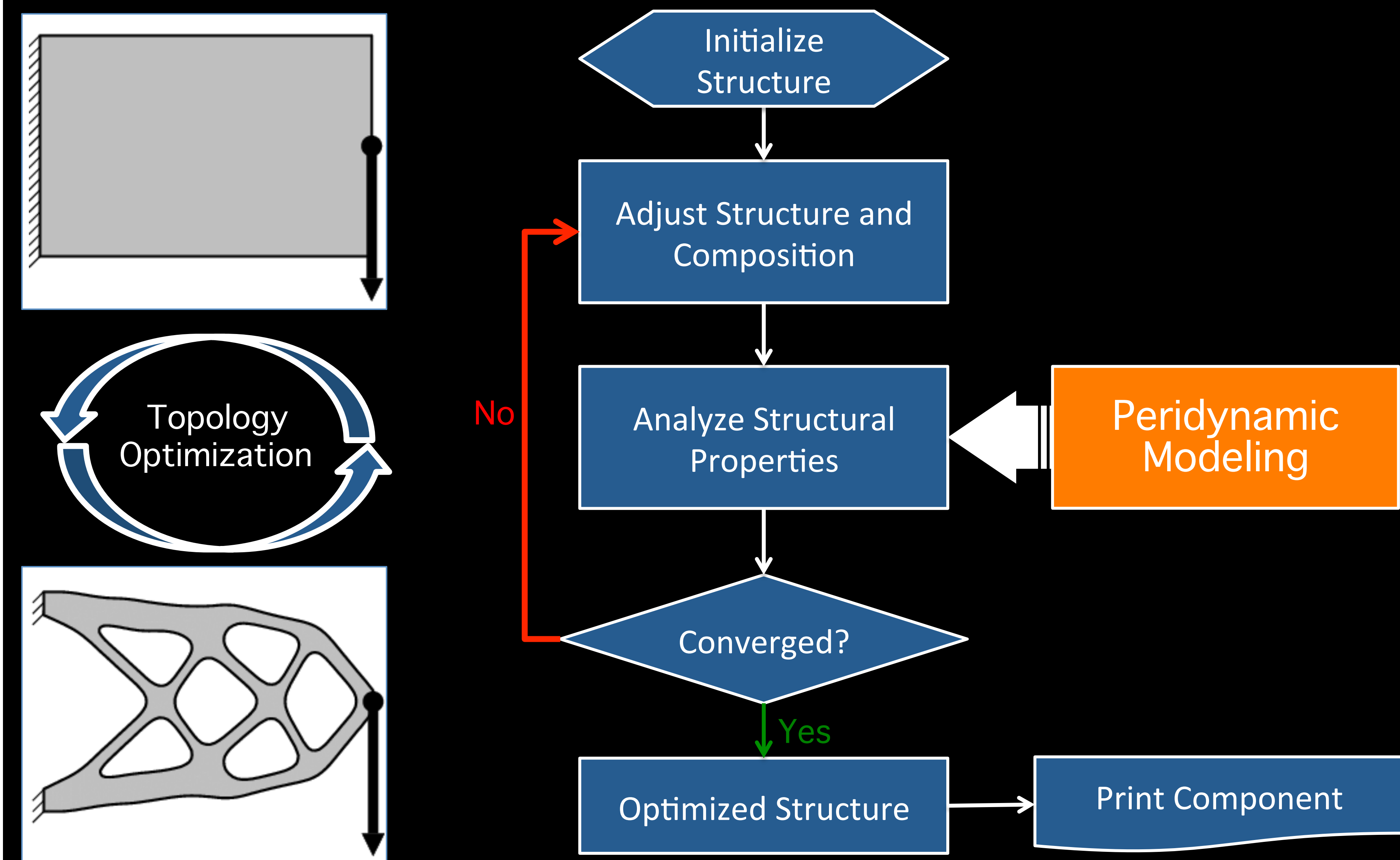
# Multiscale Modeling for CNT Composites



# Multiscale Structure of CNT Fibers



# Topology Optimization Flow Chart



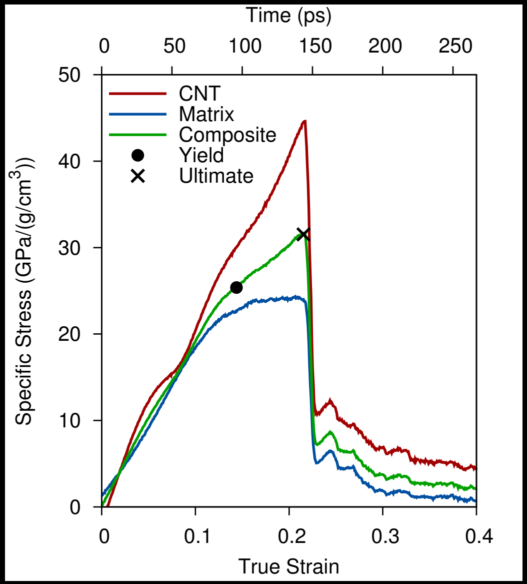
# Recent LaRC Modeling Work

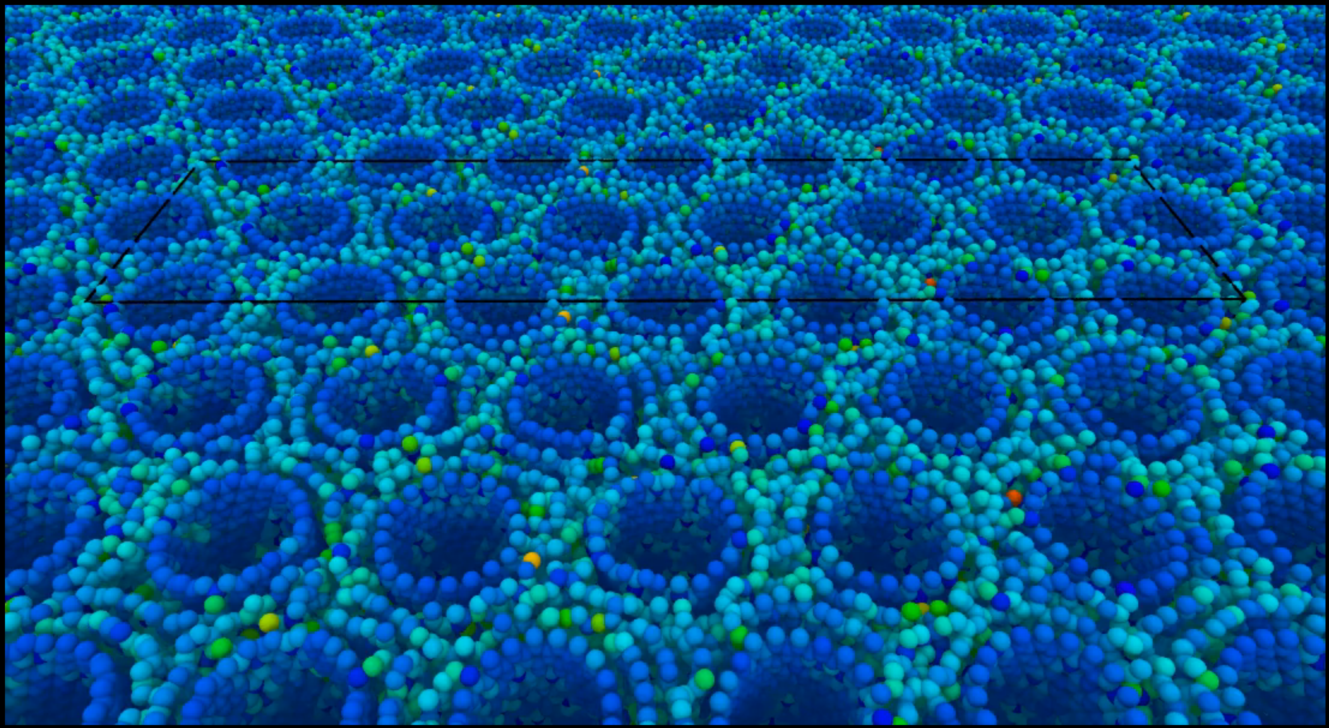
## Reactive Molecular Dynamics Simulations of CNT/Amorphous Carbon Composites

Ben Jensen, Kris Wise (LaRC)
Greg Odegard (MTU)

# Fracture of CNT Composites

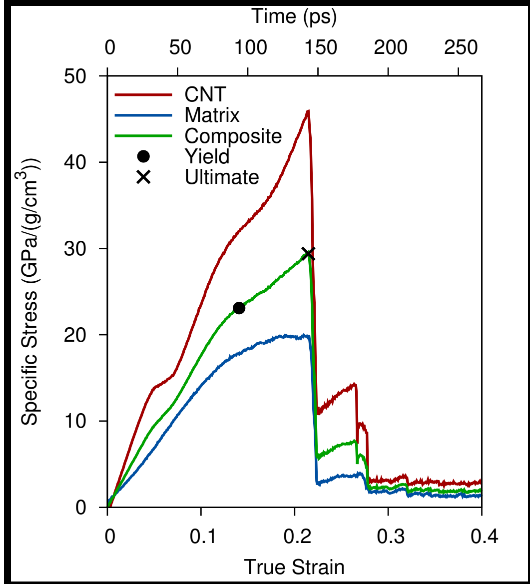
ReaxFF Simulation of a SWNT Array/Amorphous Carbon Composite

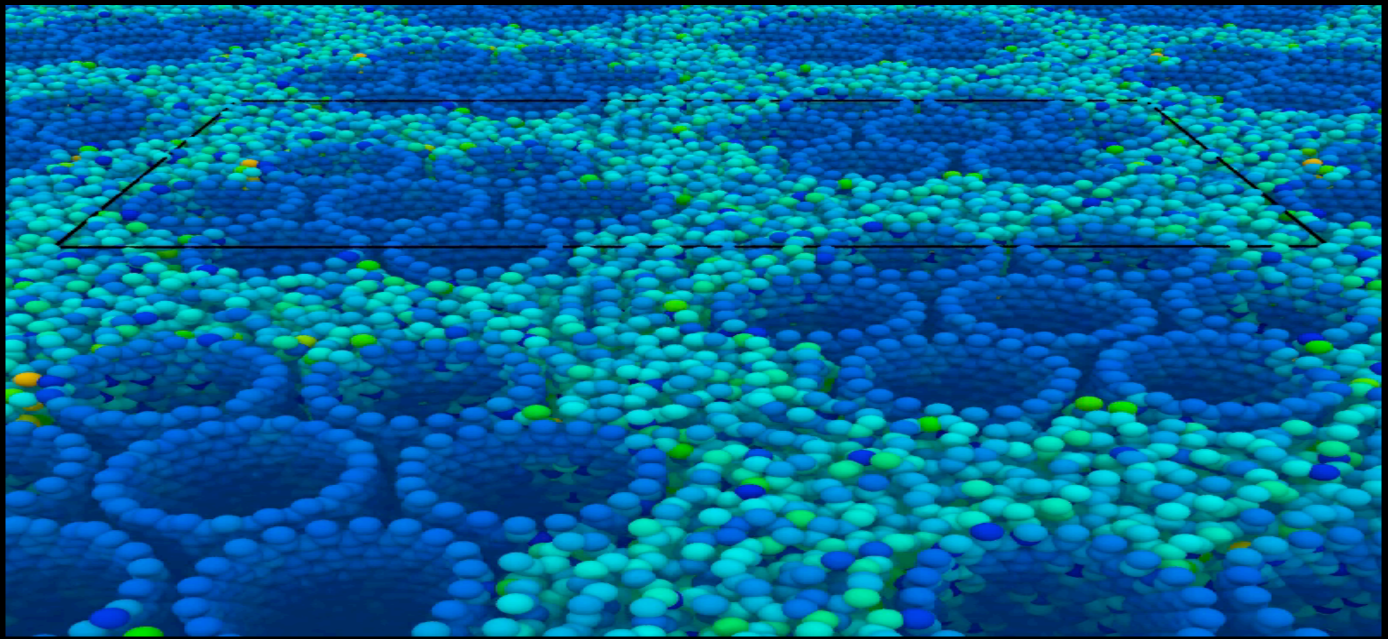


# Fracture of CNT Composites

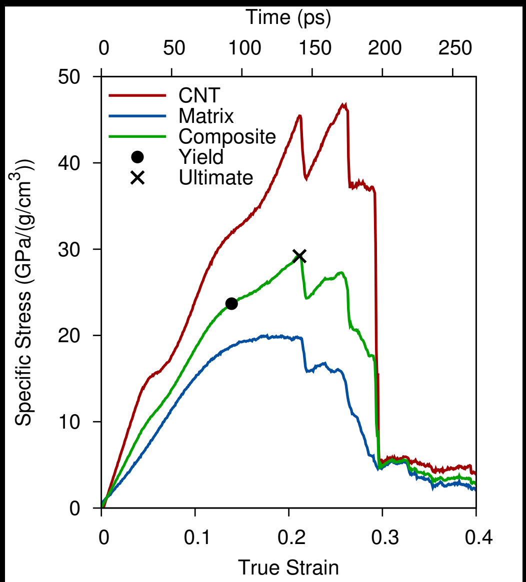
ReaxFF Simulation of a SWNT Bundle/Amorphous Carbon Composite

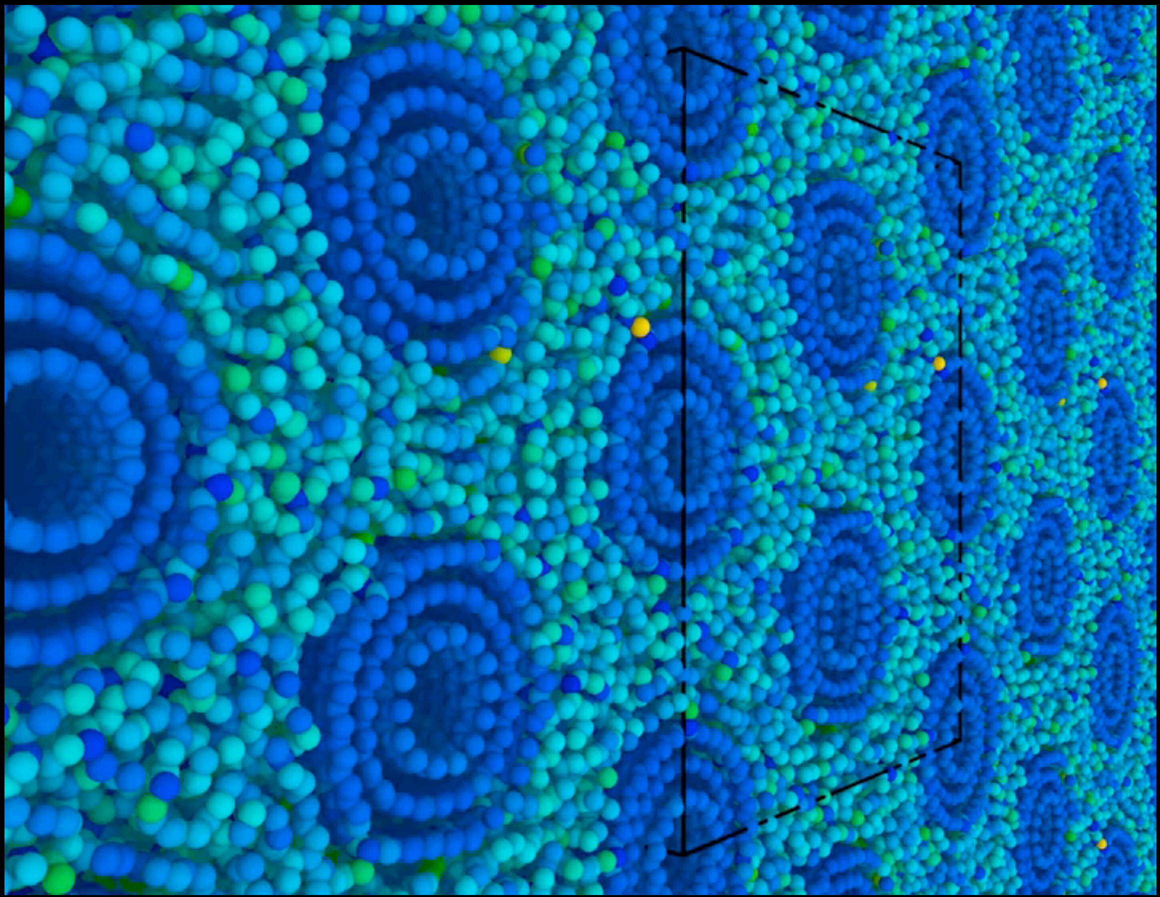


# Fracture of CNT Composites

ReaxFF Simulation of a MWNT Array/Amorphous Carbon Composite

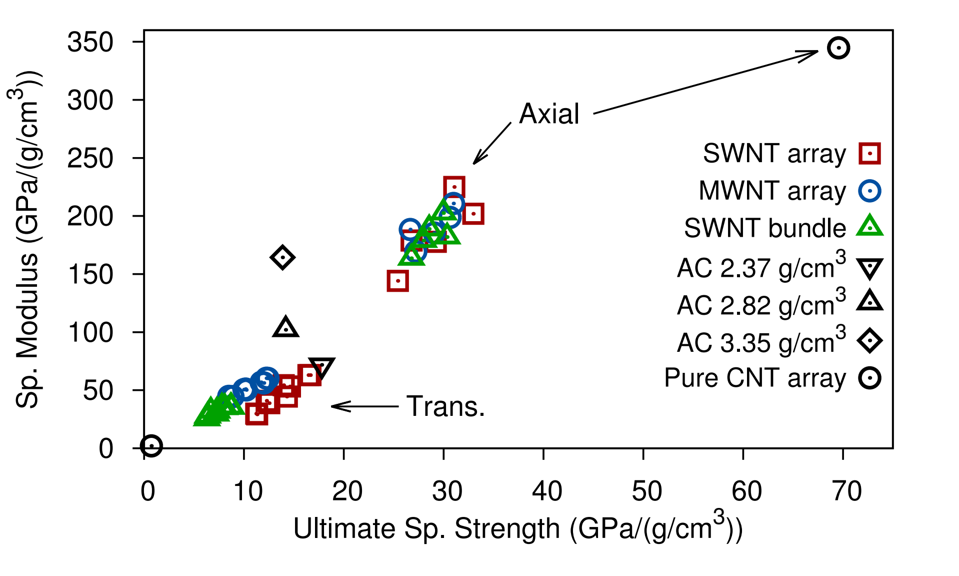


# Summary of Fracture Results

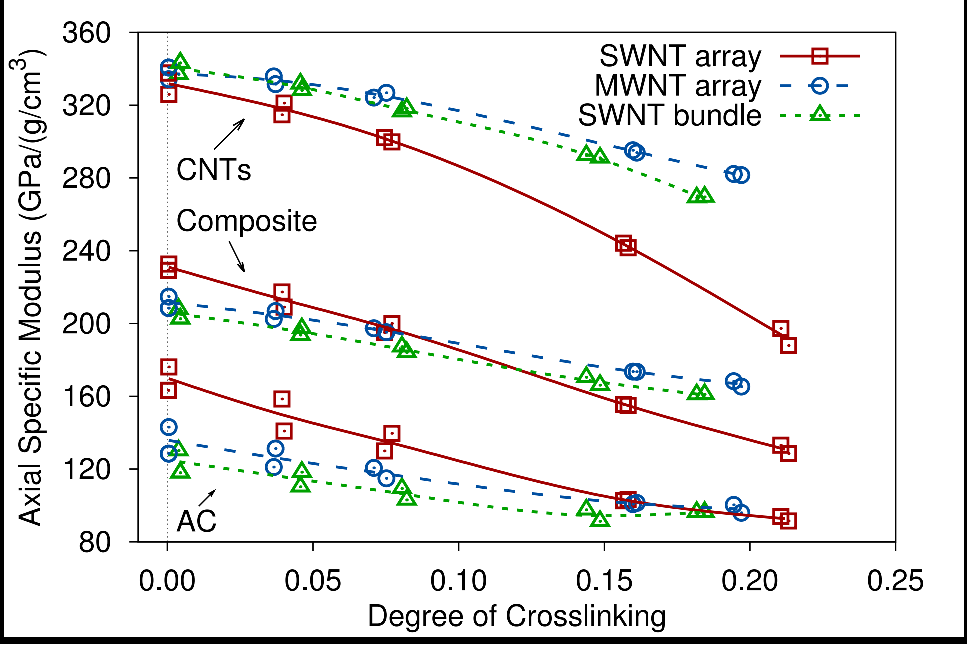
## Trends in Mechanical Properties

- Axial specific moduli ≈200 GPa, axial specific strength ≈ 30 GPa
- Transverse specific moduli ≈ 50 GPa, transverse specific strengths ≈ 10 GPa
- These results place an upper bound on expected experimental results



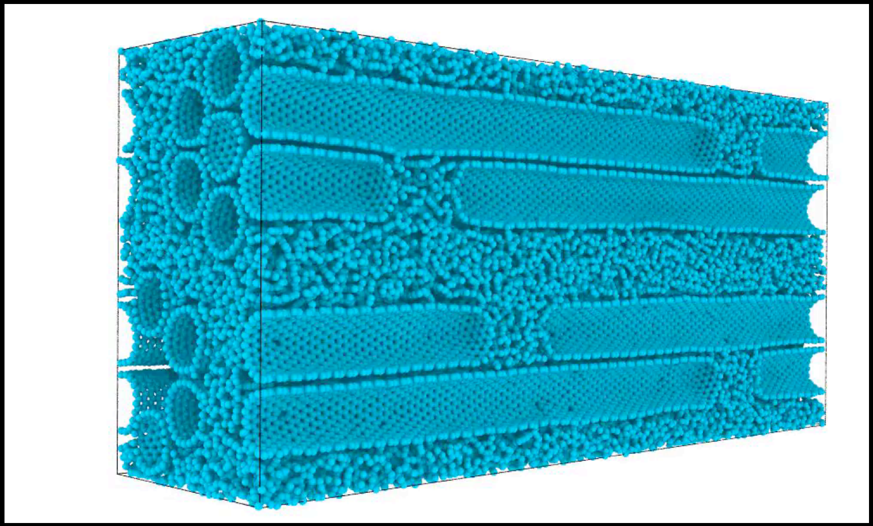

## Effect of Crosslinking to the Matrix

- SWNT Array most sensitive to crosslinking, which is reduced by bundling
- Smallest reduction in specific modulus found for MWNT array
- Loss in axial properties compensated for by increase in transverse directions

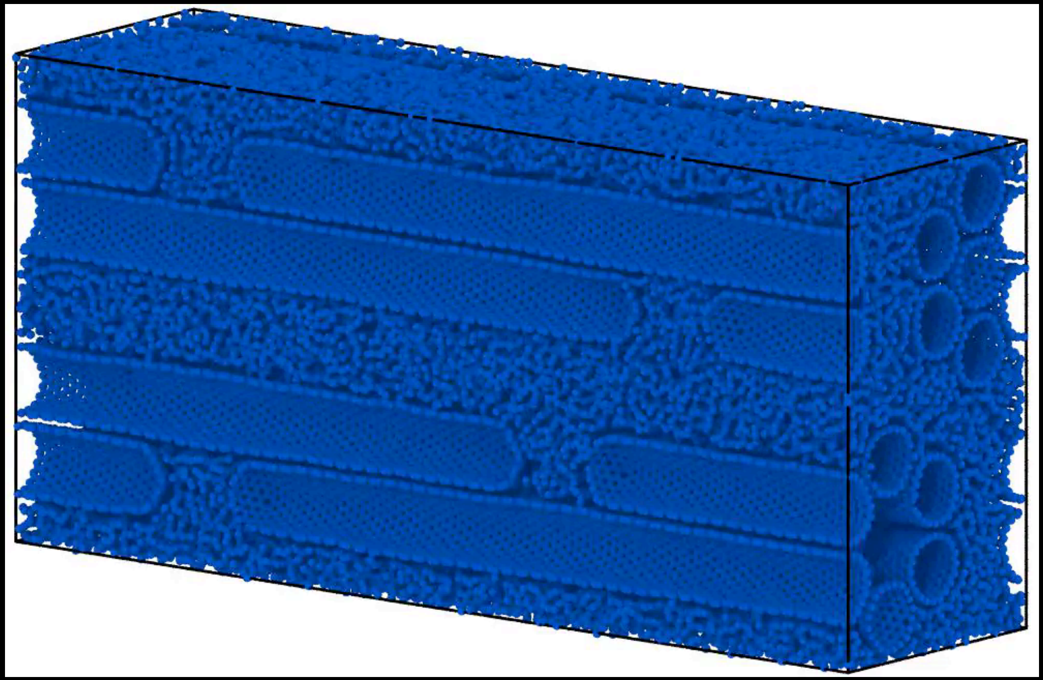


# Discontinuous SWNT Bundles

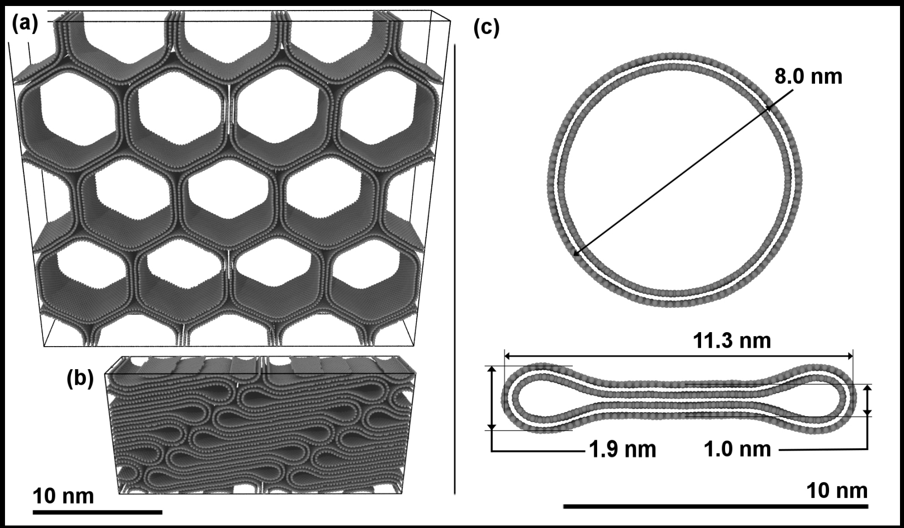
Tension

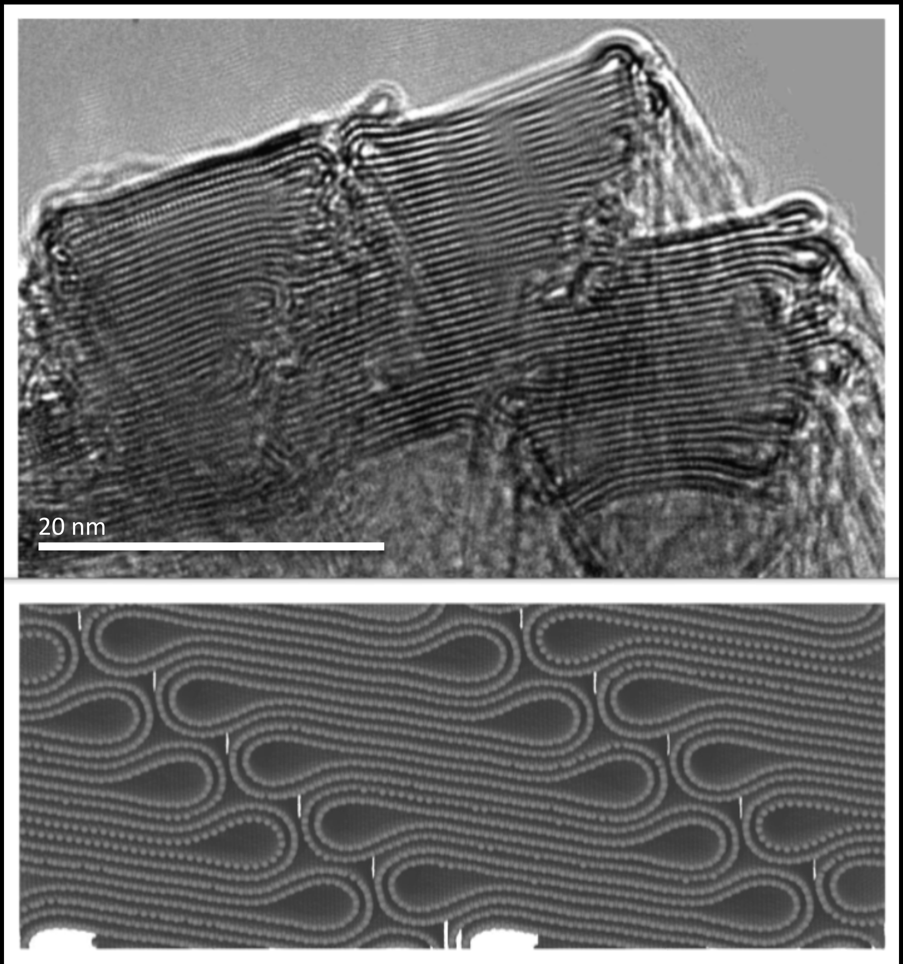


Compression



# Collapse of Large Diameter CNTs



# Acknowledgements

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